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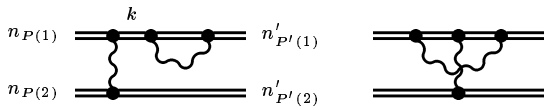
Expressions for the effective Quantum Electrodynamics (QED) Hamiltonian due to self-energy screening (self-energy correction to the electron-electron interaction) are presented. We use the method of the two-time Green's function, which handles quasidegenerate atomic states. From these expression one can evaluate energy corrections to, e.g., $1s2p\,^3P_1$ and $1s2p\,^1P_1$ in helium and two-electron ions, to all orders in $Z\alpha$.

In the last ten years, experiments in the spectroscopy of helium [1–5] have become two orders of magnitude more precise than the best theoretical energy level calculations available (see, e.g., Refs. [6,7] and references therein). Several experiments are now focusing on Helium and heliumlike ions $1s2p\,^3P_J$ fine structure [8–12], with the aim of providing a new determination of the fine structure constant and of checking higher-order effects in the calculations. In this case the theory is again a limiting factor. In this context a direct determination of all α^2 contributions to all order in $Z\alpha$ is necessary to improve reliability and accuracy of theoretical calculations (α being the fine structure constant, and Z the charge of the nucleus).

A difficulty in the study of the $(1s2p_{1/2})_1$ and $(1s2p_{3/2})_1$ levels is that they are quasidegenerate for low and middle Z ions [13]; this precludes the use of the Gell-Man–Low and Sucher method [14,15] to evaluate QED energy shifts of atomic levels. In fact, this method has two important drawbacks: it does not handle quasidegenerate energy levels, and it leads to a difficult renormalization procedure when applied to degenerate states. (The latter problem has only been tackled up to second-order in α [16,17].)

We use the method of the two-time Green's function [18–20], rigorously derived from QED (for the most detailed description of this method, see [21]). To the best of our knowledge, only the method recently proposed by Lindgren [22], closely modeled to multireference-state Many-body perturbation techniques, is designed to work for quasidegenerate states.

We evaluate the contribution of the screened self-energy diagrams



(1)

to quasidegenerate energy levels in heliumlike ions. Our results can be easily extended to ions with more than two electrons along lines similar to those found in [23].

First approximate evaluations of the contribution of these diagrams for isolated states in two- and three-electron ions were performed in Refs. [24–27]. Accurate calculations from the first principles of QED were accomplished in Refs. [28–30] for the *ground state* of *heliumlike* ions and in Refs. [31,32] for the $2s$ and $2p_{1/2}$ states of *lithiumlike* ions. The other two α^2 corrections to the electron-electron interaction have also been calculated for *isolated* states in two- and three-electron ions: the *vacuum-polarization screening* [13,29,30,33,34], and the *two-photon exchange* diagrams [35–38]. In [13], the vacuum polarization screening for quasidegenerate states of heliumlike ions was evaluated as well. Some results for the direct contribution of the self-energy correction to the Coulomb interaction are also available [24,39].

As depicted in diagrams (1), the interaction between the two electrons through photons is treated perturbatively. On the contrary, the binding to the nucleus is included *non-perturbatively* in the method we use, since the corresponding coupling constant is $Z\alpha$. Such a treatment is obviously mandatory for highly-charged ions. Furthermore, it allows one to compare non-perturbative (in $Z\alpha$) results to (semi-)analytic expansions in $Z\alpha$ (see [40] for a review).

We derive the effective (finite-sized) matrix hamiltonian H, whose eigenvalues give the contribution of QED to a group of energy levels [23]. The diagonal entries of the hamiltonian that we evaluate correctly reproduce previous expressions of the screened self-energy, while the new, non-diagonal entries that we derive allow one to obtain a second-order QED correction to *quasidegenerate* or *degenerate* energy levels.

Relativistic units $\hbar = c = 1$ are used throughout this paper.

If we have s quasidegenerate energy levels $E^{(0)}_{1\ldots s}$, the effective hamiltonian H is an $s \times s$ matrix restricted to these levels [23]. Let us introduce some notations in order to express this hamiltonian. The second-order contribution $H^{(2)}$

to this hamiltonian $H = H^{(0)} + H^{(1)} + H^{(2)} + \ldots$ is constructed from a projection matrix P and an energy matrix K [23]:

$$H^{(2)} = K^{(2)} - \frac{1}{2}\{P^{(1)}, K^{(1)}\} - \frac{1}{2}\{P^{(2)}, K^{(0)}\} + \frac{3}{8}\{[P^{(1)}]^2, K^{(0)}\} + \frac{1}{4}P^{(1)}K^{(0)}P^{(1)}, \tag{2}$$

where the notation $\{,\}$ represents the usual anticommutator, and where the superscripts indicate the number of photons of the diagrams that contribute to each term of the perturbative expansion $P = P^{(0)} + P^{(1)} + \ldots$ and $K = K^{(0)} + K^{(1)} + \ldots$; the $s \times s$ matrices P and K, which are defined as [20]:

$$P \equiv \frac{1}{2\pi i}\oint_\Gamma dE\, g(E) \tag{3a}$$

$$K \equiv \frac{1}{2\pi i}\oint_\Gamma dE\, E\, g(E), \tag{3b}$$

where $g(E)$ is the $s\times s$ matrix restriction of the Green's function to the s unperturbed atomic levels under consideration, and where Γ is a contour that encloses each of the Dirac atomic energy levels with a positive orientation [23].

We directly evaluate the hamiltonian matrix elements of Eq. (2) between states of *different* energies $E_n^{(0)}$ and $E_{n'}^{(0)}$, and put them in a form that readily displays the limiting case of *identical* energies; we checked by a direct calculation of the diagonal matrix elements that they can be obtained from non-diagonal elements $H^{(2)}_{nn'}$ by taking the formal limit $E_n^{(0)} \to E_{n'}^{(0)}$. *All* the subsequent derivations of $H^{(2)}_{nn'}$ will thus be done with $E_n^{(0)} \neq E_{n'}^{(0)}$.

The first diagram of (1) appears only in the second-order matrices $K^{(2)}$ and $P^{(2)}$ in Eq. (2). As usual, we must calculate a *reducible* and an *irreducible* contribution; as can be seen in subsequent calculations, it turns out that the correct extension of these notions to quasidegenerate states is the following: in the first diagram of Eq. (1), the contribution of intermediate electrons with a Dirac energy ε_k such that $\varepsilon_k + \varepsilon_{n'_{P'(2)}}$ coincides with one of the s energy levels under consideration and must be *separated out* from the contribution of the other intermediate electron states; the first contribution (called *reducible*) requires a different mathematical treatment from that of the second contribution (called *irreducible*).

Thus, the *irreducible* contribution is obtained by summing over almost all electron states k in the first diagram of Eq. (1); we first show that it is sufficient to remove only *one* state k from the sum over states in the first diagram of Eq. (1). We see that an intermediate energy $\varepsilon_k + \varepsilon_{n'_{P'(2)}}$ can coincide with an unperturbed atomic levels $E^{(0)}_{1\ldots s}$ only if the electron k has the *same principal quantum number* as the electron $n'_{P'(1)}$ on the other side of the self-energy, because otherwise the total energy $\varepsilon_k + \varepsilon_{n'_{P'(2)}}$ would lie largely out of the range spanned by the unperturbed quasidegenerate energy levels located around $E^{(0)}_{n'} = \varepsilon_{n'_{P'(1)}} + \varepsilon_{n'_{P'(2)}}$.

There is an additional selection on the electrons k to be removed: since the total angular momentum, its projection, and parity are conserved by the self-energy operator Σ [Eq. (6) below], as can be seen by integrating over angles using standard techniques [41], the contribution of electrons k that do not share the same quantum numbers (κ, m) as the electron $n'_{P'(1)}$ in the first diagram of Eq. (1) is exactly *zero*.

We denote the individual electrons of a state n by n_1 and n_2, in an order which is arbitrary but that must remain fixed. With these notations, our evaluation of the *irreducible* part of the first diagram of (1) to the effective hamiltonian (2) takes a simple form and reads (Dirac energies are still denoted by ε_k):

$$\begin{aligned} H^{\text{scr. SE, irr.}}_{nn'} = \sum_{P,P'} (-1)^{PP'} \Bigg(& \sum_{k\neq n_{P(1)}} \langle n_{P(1)}|\Sigma(\varepsilon_{n_{P(1)}})|k\rangle \frac{1}{\varepsilon_{n_{P(1)}} - \varepsilon_k} \langle k n_{P(2)}|I(\varepsilon_{n_{P(1)}} - \varepsilon_{n'_{P'(1)}})|m'_1 m'_2\rangle \\ & + \sum_{k\neq n'_{P'(1)}} \langle n_{P(1)} n_{P(2)}|I(\varepsilon_{n_{P(1)}} - \varepsilon_{n'_{P'(1)}})|n'_{P'(1)} n'_{P'(2)}\rangle \frac{1}{\varepsilon_{n'_{P'(1)}} - \varepsilon_k} \langle k|\Sigma(\varepsilon_{n'_{P'(1)}})|n'_{P'(1)}\rangle \Bigg) \\ & + \mathcal{O}[\alpha^2(E^{(0)}_{n'} - E^{(0)}_n)], \end{aligned} \tag{4}$$

where $(-1)^{PP'}$ is the signature of the permutation $P \circ P'$ (P and P' are permutations of $\{1, 2\}$.), where the sum over k is over (almost) all possible intermediate Dirac states, and where the photon exchange and the self-energy of diagrams (1) are represented by the following usual operators [32]:

$$\langle ab|I(\omega)|cd\rangle \equiv e^2 \int d^3\boldsymbol{x}_1 \int d^3\boldsymbol{x}_2 \, [\psi_a^\dagger(\boldsymbol{x}_1)\alpha^\mu\psi_c(\boldsymbol{x}_1)] \times[\psi_b^\dagger(\boldsymbol{x}_2)\alpha^\nu\psi_d(\boldsymbol{x}_2)]D_{\mu\nu}(\omega;\boldsymbol{x}_1-\boldsymbol{x}_2) \tag{5}$$

$$\langle a|\Sigma(p)|b\rangle \equiv \frac{1}{2\pi i}\int d\omega \sum_k \frac{\langle ak|I(\omega)|kb\rangle}{\varepsilon_k(1-i0)-(p-\omega)}, \tag{6}$$

in which e is the charge of the electron, $\alpha^\mu \equiv (1,\boldsymbol{\alpha})$ are the Dirac matrices, and where ψ denotes a Dirac spinor; the photon propagator D is given in the Feynman gauge by

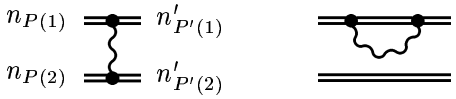
$$D_{\nu\nu'}(\omega;\boldsymbol{r}) \equiv g_{\nu\nu'}\frac{\exp\left(i|\boldsymbol{r}|\sqrt{\omega^2-\mu^2+i0}\right)}{4\pi|\boldsymbol{r}|}, \tag{7}$$

where μ is a small photon mass that eventually tends to zero, and where the square root branch is chosen such as to yield a decreasing exponential for large real-valued energies ω.

The last term in Eq. (4) represents a contribution of order α^2 which is multiplied by a factor that tends to zero as $E^{(0)}_{n'} - E^{(0)}_n \to 0$. It can be shown (see Ref. [21]) that such a term does not contribute to order α^2 and that it can therefore be omitted.

We note that result (4) readily yields diagonal elements by taking the (formal) limit $E^{(0)}_n - E^{(0)}_{n'} \to 0$.

The hamiltonian (2) contains the contribution of many *first*-order diagrams through the operators $P^{(1)}$ and $K^{(1)}$. We must consider here the contribution of the photon exchange and of the self-energy



; (8)

their contribution to Eq. (2) *cancels* a part of the *reducible* screened self-energy. We thus evaluate in the following the contribution of both diagrams of Eq. (8) to the terms $-\frac{1}{2}\{P^{(1)},K^{(1)}\} + \frac{3}{8}\{[P^{(1)}]^2,K^{(0)}\} + \frac{1}{4}P^{(1)}K^{(0)}P^{(1)}$ of the effective hamiltonian.

The energy and projection matrices K and P of Eq. (3) have been calculated for the photon-exchange diagram in [13]; this allows one to evaluate any integral due to the *photon exchange* that appears in the effective hamiltonian (2).

In order to derive the contribution of the *one-electron* self-energy, let us show that the evaluation of the self-energy contributions to the hamiltonian (2) boils down to the calculation of contour integrals of the form

$$\frac{1}{2\pi i}\oint_{\Gamma_n} dE\, g^{\rm SE}_{nn}(E) \quad \text{and} \quad \frac{1}{2\pi i}\oint_{\Gamma_n} dE\, E\, g^{\rm SE}_{nn}(E) \tag{9}$$

where $g^{\rm SE}_{nn}(E)$ are diagonal elements of the self-energy Green's function; in other words, the contour Γ that surrounds *all* the levels in Eq. (3) can be replaced by the contour that surrounds $E^{(0)}_n$ *only*, and *non-diagonal* elements of the self-energy Green's function are not relevant. The contour integrals of Eq. (9) have both been evaluated in [32], so that no further quantity is required in order to obtain the self-energy contribution to the hamiltonian (2).

Let us prove the above statements. As mentioned before, angular momentum conservations constrain the self-energy operator Σ to be zero between states with different angular quantum numbers (κ, m); and since the atomic levels we consider have the same principal quantum number (they are quasidegenerate), the self-energy Green's matrix is diagonal:

$$g^{\rm SE}_{nn'}(E) = 0 \quad \text{if } n \neq n', \tag{10}$$

where n and n' are the *sets* of quantum numbers of two of the s levels under consideration.

Furthermore, the Green's function $g^{\rm SE}_{nn}(E)$ has only *one* pole inside the integration contour Γ, namely at $E = E^{(0)}_n$. Therefore, integrating over the full contour Γ in the hamiltonian (2) amounts to integrate over the contour Γ_n that surrounds only $E^{(0)}_n$, since the Green's function is analytic inside the contours that encircle the other energies.

We thus see that the contribution of the self-energy to Eq. (2) depends only on contour integrals of the form (9), which are known analytically [32].

With the help of some published analytical formulas, we obtain the following contribution of the photon exchange (see Eqs. (27) and (28) in [13]) and of the self-energy (see Eqs. (36) and (37) in [32]) to the effective hamiltonian (2):

$$
-\sum_{P,P'}(-1)^{PP'}\left\{\frac{1}{4}\Bigg[\Big(\langle n_{P(1)}|\Sigma'(\varepsilon_{n_{P(1)}})|n_{P(1)}\rangle+\langle n'_{P(1)}|\Sigma'(\varepsilon_{n'_{P(1)}})|n'_{P(1)}\rangle\Big)\right.
$$

$$
\left.\times\Big(\langle n_{P(1)}n_{P(2)}|I(\Delta_1)|n'_{P'(1)}n'_{P'(2)}\rangle+\langle n_{P(1)}n_{P(2)}|I(\Delta_2)|n'_{P'(1)}n'_{P'(2)}\rangle\Big)\Bigg]\right.
$$

$$
+\frac{1}{2}\Bigg[\Big(\langle n_{P(1)}|\Sigma(\varepsilon_{n_{P(1)}})|n_{P(1)}\rangle+\langle n'_{P(1)}|\Sigma(\varepsilon_{n'_{P(1)}})|n'_{P(1)}\rangle\Big)
$$

$$
\left.\times\frac{1}{2\pi i}\int d\omega\,\langle n_{P(1)}n_{P(2)}|I(\omega)|n'_{P'(1)}n'_{P'(2)}\rangle\left(\frac{1}{(\omega+\Delta_1-i0)(\omega-\Delta_2-i0)}+\frac{1}{(\omega+\Delta_2-i0)(\omega-\Delta_1-i0)}\right)\Bigg]\right\}, \quad (11)
$$

where Σ' represents the derivative of the self-energy operator (6) with respect to the energy that flows in it, and where the two possible energies for the photon in the photon-exchange diagram are $\Delta_1 \equiv \varepsilon_{n_{P(1)}} - \varepsilon_{n'_{P'(1)}}$ and $\Delta_2 \equiv \varepsilon_{n_{P(2)}} - \varepsilon_{n'_{P'(2)}}$.

As seen above, the *reducible* part of the *first* diagram of Eq. (1) represents the contribution of an intermediate electron $k = n'_{P'(1)}$. (For the *second* diagram, the reducible part is similarly obtained through an intermediate electron $k = n_{P(1)}$.) The evaluation of the reducible contribution follows steps similar to those used for the irreducible part. The contribution of diagrams (8) to the effective hamiltonian $H^{(2)}$, which is given in Eq. (11), *cancels* a few terms of the contribution of the reducible diagram, as for diagonal matrix elements [32]; the total *reducible* contribution to Eq. (2) is then found to be:

$$
H^{\text{scr. SE, red.}}_{nn'} = \sum_{P,P'}(-1)^{PP'}\frac{1}{2}\Bigg[\partial_p|_{\varepsilon_{n_{P(1)}}}\Big(\langle n_{P(1)}|\Sigma(p)|n_{P(1)}\rangle\langle n_{P(1)}n_{P(2)}|I(p-\varepsilon_{n'_{P'(1)}})|n'_{P'(1)}n'_{P'(2)}\rangle\Big)
$$

$$
+\partial_{p'}|_{\varepsilon_{n'_{P'(1)}}}\Big(\langle n_{P(1)}n_{P(2)}|I(\varepsilon_{n_{P(1)}}-p')|n'_{P'(1)}n'_{P'(2)}\rangle\langle n'_{P'(1)}|\Sigma(p')|n'_{P'(1)}\rangle\Big)\Bigg]
$$

$$
+\mathcal{O}[\alpha^2(E^{(0)}_{n'}-E^{(0)}_{n})], \quad (12)
$$

where $\partial_x|_{x_0}$ represents the derivative with respect to x at the point x_0.

For the vertex diagram [second diagram of (1)], the two-time Green's function method yields the following contribution to (2):

$$
H^{\text{vertex}}_{nn'} = \sum_{P,P'}(-1)^{PP'}\sum_{i_1,i_2}\langle i_1 n_{P(2)}|I(\varepsilon_{n_{P(1)}}-\varepsilon_{n'_{P'(1)}})|i_2 n'_{P'(2)}\rangle
$$

$$
\times\frac{i}{2\pi}\int d\omega\,\frac{\langle n_{P(1)}i_2|I(\omega)|i_1 n'_{P'(1)}\rangle}{[\varepsilon_{i_1}(1-i0)-(\varepsilon_{n_{P(1)}}-\omega)][\varepsilon_{i_2}(1-i0)-(\varepsilon_{n'_{P'(1)}}-\omega)]}+\mathcal{O}[\alpha^2(E^{(0)}_{n'}-E^{(0)}_{n})], \quad (13)
$$

with the same notations as before; the sum is over all pairs of Dirac states.

We thus have obtained the full contribution [Eq. (4) + Eq. (12)+Eq. (13)] of the screened self-energy diagrams (1) to a finite-sized effective hamiltonian which acts on a few atomic energy levels (in the general case: quasidegenerate, fully degenerate or isolated); the eigenvalues of this hamiltonian give the QED prediction for the energy levels. We have also taken into account the contribution of the first-order diagrams (8) to the second-order hamiltonian (2).

The results presented here extend previous derivations of the screened self-energy contribution to the Lamb shift, which were restricted to the evaluation of the energy shift of an *isolated* level. The diagonal terms of the effective hamiltonian that we have evaluated confirm previously published results. The new, non-diagonal matrix elements of the hamiltonian that we obtained allow one to calculate the energy shifts of quasidegenerate levels and to extend numerical calculations [24,28–31,42] to such levels.

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